Velocity and diffusion coefficient of $A+A \leftrightarrow A$ reaction fronts in one dimension

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We study front propagation in the reversible reaction-diffusion system $A+A \leftrightarrow A$ on a one-dimensional lattice. Extending the idea of *leading* particle in studying the motion of the front we write a master equation in the stochastically moving frame attached to this particle. This approach provides a systematic way to improve on estimates of front speed obtained earlier. We also find that the leading particle performs a correlated random walk and this correlation needs to be taken into account to get the correct the value of the front diffusion coefficient.

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I. INTRODUCTION

Propagation of fronts into unstable states in reaction-diffusion systems has been an actively studied topic for a long time [1]. The dynamics of propagating fronts is of interest in diverse physical situations—for example, on a binary search tree in computer science [2], the front between zipped and unzipped phases on DNA [3], solidification front [4], flame front in air-fuel mixture [5], etc. Recently, there has been renewed activity concerning the connection between fronts in microscopic discrete stochastic models and macroscopic deterministic equations which are believed to be their mean-field limits [6]. In this paper we study front propagation in a system of reacting and diffusing particles on an infinite one-dimensional (1D) lattice. Initially, the left half of the lattice is filled with a certain density of particles with the right half being completely empty, resulting in a sharp boundary between the two halves. As the system evolves, the particles move to the right, resulting in a propagating front. After an initial transient, the front moves with an asymptotic speed v. Further, due to the inherent stochastic nature of the dynamics, the ensemble-averaged front profile in the lattice frame undergoes diffusive broadening [Fig. 1(a)] with an associated diffusion coefficient D_f. However, if the ensemble average is taken in a frame moving with the rightmost particle (the *leading* particle) in each realization, the density profile does not change in time [Fig. 1(b)] and is microscopically sharp (i.e., a few lattice spacing wide). Thus, the diffusive spreading of the profile in the fixed frame is entirely due to the random motion of the leading particle. This indicates that the dynamics of the front is reduced, in an approximate way, to the dynamics of the leading particle [7–9]. Treating the motion of this particle as a biased random walk, simple approximate expressions for the speed v and diffusion coefficient D_f have been derived [8,9]. However, in these approaches it is hard to find a systematic way to improve estimates for v and D_f. In the present paper we show that by writing the front dynamics in the frame moving with the leading particle one can get numerically better estimates of the front speed. We also show that the motion of the leading particle is correlated in time and thus the front diffusion coefficient differs from that obtained from a simple random-walk approximation.

II. MODEL AND RESULTS FOR v AND D_f

We consider a 1D lattice $(-\infty < i < \infty)$ in which each site can hold at most one particle (hard-core exclusion). The particles (denoted by A) undergo three basic microscopic processes: (i) Birth or creation: a particle can generate a new one on a neighboring empty site with rate ϵ. (ii) Death or annihilation: one of the two neighboring particles gets annihilated with rate W (iii) Diffusion: a particle diffuses to a neighboring empty site with rate D (see Fig. 2). Initially, at $t=0$, the left half of the lattice $(i \leq 0)$ is filled with particles at a density $\rho=\bar{\rho}$, where $\bar{\rho}=\epsilon/(\epsilon+W)$ is the density of the equilibrium phase eventually obtained if the process were allowed to occur in a finite system. There are only two independent parameters in the system as one of the three rates ϵ, D, and W can be scaled away by choosing the time scale appropriately.

In a mean-field approach, which is expected to be valid in the limit $D \to \infty$, the evolution of the front is described by the Fisher-Kolmogorov-Petrovsky-Piskunov (FKPP) equation [10] $\partial_t \rho = D\partial_x^2 \rho + k_1 \rho - k_2 \rho^2$, with $k_1=2\epsilon$, $k_2=2(\epsilon+W)$, and ρ is the coarse-grained density of A particles. The asymptotic front speed is then given by $v_0=2\sqrt{2\epsilon D}$.

For the case $W=0$, which arises naturally in the context of turbulent flame-front propagation [7], the existence and uniqueness of an asymptotic front solution were established rigorously in [11] and it was shown that the mean-field limit is obtained as $D \to \infty$. For finite values of D, a two-particle representation was used in [8] to get an approximate value of the front speed which works quite well for $D/\epsilon \sim O(1)$.

In [12], using the inter particle distribution functions, an exact solution was obtained for the special case $W=D$. In this case, it was shown that in each realization of the front evolution, the leading particle performs a biased random walk and the spatial distribution of particles behind is the same as in equilibrium with density $\rho=\bar{\rho}$. The speed and diffusion coefficient in this case are $v=\epsilon$ and $D_f=\epsilon+D$, respectively.

If $W \neq D$, the method used in [12] does not work and an exact solution is no longer possible. Also, the two-particle representation of [8] does not close if particle annihilation is introduced—i.e., $W>0$. In [9], an approach based explicitly on the motion of the leading particle as a biased

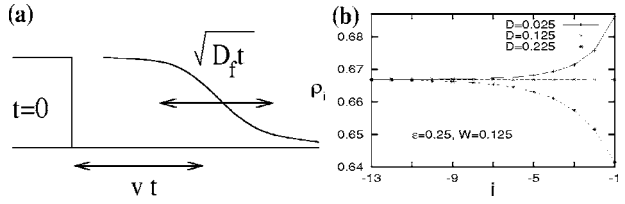

FIG. 1. Spatial density profile of the front (a) Schematic picture of the average profile (in the fixed frame) moving and spreading diffusively. (b) Numerically obtained average profiles as seen from the frame of the rightmost particle for three different sets of parameters defined in the text. The right edge of the graph ($i=-1$) corresponds to the site just behind the leading particle.

random walker was introduced and the following approximate expressions for speed and diffusion coefficient were obtained:

$$v = \epsilon - \rho_1(W-D), \quad 2D_f = 2D + \epsilon - \rho_1(W-D), \qquad (1)$$

where ρ_1 is the probability of occupation of the site just behind the leading particle. Expression (1) may be written down by noting that the front particle moves right with rate $\epsilon+D$ (i.e., whenever a particle is created to the right of the leading particle or the later makes a diffusive move to the right). The leading particle takes a negative step when it gets annihilated by the particle on the left (with rate $W\rho_1$) or if it makes a diffusive move to an empty left site [with rate $D(1-\rho_1)$], where ρ_1 is the occupation probability of the site immediately to the left of the leading particle. For $W=D$, these results reduce to those obtained exactly in [12]. In order to get more accurate values of v and D_f one needs to find better estimates of ρ_1 (the bulk value $\rho_1=\bar{\rho}$ was used in [9]). While Eq. (1) works quite well (with $\rho_1=\bar{\rho}$) for W close to D, there are significant deviations as one moves away from this special point ($W=D$). This can be seen from Fig. 1(b) where ρ_1 is significantly different from $\bar{\rho}$ for $|W-D|>0$. Here we present the results of simulations for two different sets of parameters ($\epsilon=0.25, W=0.125$) and ($\epsilon=0.05, W=0.0$) while varying D in each set. The second set allows for the largest possible deviation from the $D=W$ special point.

In order to get successively better estimates for ρ_1, we look at the invariant profile of the front as observed from the leading particle. Starting from an ensemble of $\mathcal{N}$ realizations this invariant profile is obtained, after an initial transient time, by aligning the leading particle of each member of the ensemble [Fig. 1(b)]. From the definition of ρ_1 it then follows that out of the $\mathcal{N}$ realizations, $\rho_1\mathcal{N}$ have a particle in the site to the left of the leading particle and the rest $(1-\rho_1)\mathcal{N}$ have an empty site next to it. In the steady state, it thus follows that there is a kinetic balance between the two types of realizations: those with 11 or 01 as the occupancy of the rightmost pair of sites (where the second 1 denotes the leading particle). Thus, the two states 01 and 11 may be thought of as a truncated representation of the full lattice. Due to microscopic moves, there are transitions between these two "states." In this representation the state may not always change although the configuration of the lattice as a whole

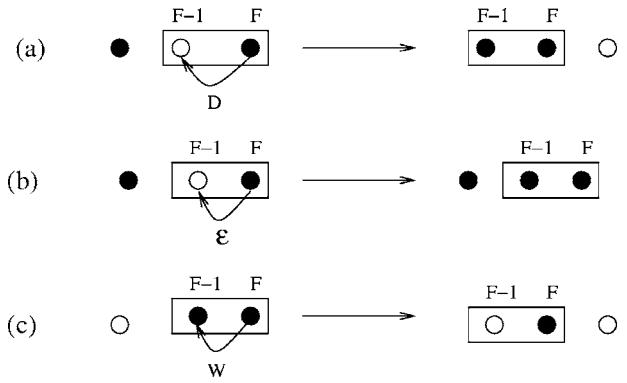

FIG. 2. Basic microscopic moves of (a) diffusion, (b) birth, and (c) death. When the right particle happens to be the leading particle (denoted by F) the processes can result in transitions between the two states 01 and 11 as described later in the text.

changes. E.g., in the 11 state if a new particle is created to the right of the leading particle, the state remains as 11. For example, in the transition shown in Fig. 2(b), the configuration 01 changes to 11 with rate ϵ. In Fig. 2(a), diffusion of the leading particle to its left changes the state 01→11 provided the site F-2 is occupied and leaves it unchanged if F-2 is empty. If the probability of occupancy of F-2 is denoted by ρ_b, then the transition 01→11 occurs with the rate $D\rho_b$.[1] Similarly, in Fig. 2(c), when the leading particle in state 11 gets annihilated, the state changes to 01 if F-2 is empty and this occurs with rate $W(1-\rho_b)$. Considering all such transitions involving the leading particle and two sites behind it, one can write a master equation for the probabilities p_{11} and p_{01} of the two states in this truncated state space as

$$\dot{p}_{01} = (2D - D\rho_b + 2W)p_{11} - (2D\rho_b + 2\epsilon + \epsilon\rho_b)p_{01},$$

$$\dot{p}_{11} = (2D\rho_b + 2\epsilon + \epsilon\rho_b)p_{01} - (2D - D\rho_b + 2W)p_{11}. \qquad (2)$$

In the steady state $\dot{p}_{01}=0=\dot{p}_{11}$ and one obtains ($p_{11}=\rho_1$ in steady state)

$$\rho_1 = \frac{3\epsilon^2 + 2\epsilon(W+D)}{3\epsilon^2 + 2W^2 + 4\epsilon W + 3D\epsilon + 2DW}, \qquad (3)$$

where we have used $\rho_b=\bar{\rho}$, an approximation which becomes better as one includes more sites in the truncated representation. E.g., we have also computed ρ_1 by keeping $l=3$ sites (i.e., four states 111, 011, 101, 001), $l=4$ sites (eight states), and the relative errors in the values obtained for ρ_1 are plotted in Fig. 3 and the corresponding front speed [using Eq. (1)] in Fig. 4. It is to be noted that expression (3) above reduces to $\rho_1=\bar{\rho}$ for $W=D$ as it should. In fact our approximation $\rho_b=\bar{\rho}$ becomes exact for $W-D=0$; however, for increasing values of $|W-D|$, ρ_b differs significantly form $\bar{\rho}$

[1]Here we assume the third site is occupied with probability ρ_b, independent of whether the second site is occupied or not. This approximation is expected to become better as one includes a larger number of sites in the representation: the correlation between the last site of the truncated state and the site behind that vanishes as one approaches the bulk.

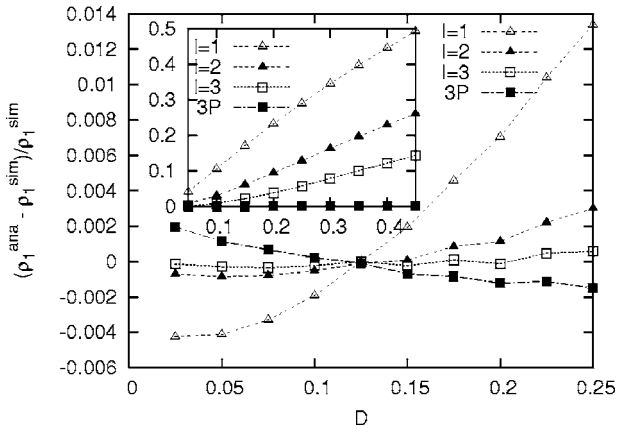

FIG. 3. Deviation of ρ_1 computed via various approximations from that obtained from direct simulation as a function of D for $W=0.125$ and $W=0$ (inset). Solid squares correspond to the three-particle representation discussed in Sec. II A.

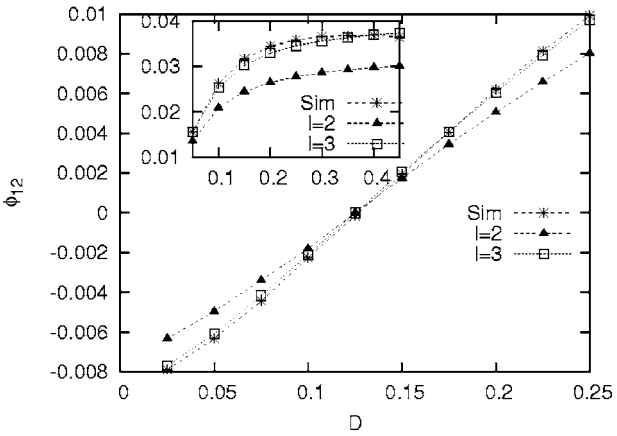

FIG. 5. The correlation ϕ_{12} between occupancies of the pair of sites immediately following the leading particle as a function of D ($W=0.125$). We see that the correlation is negative for $D<W$ and positive for $D>W$. Inset: ϕ_{12} as a function of D for $W=0$.

[Fig. 1(b)] and thus we need to study the states corresponding to larger values of l (as obvious from Figs. 3 and 4). Further, in this approach, it is also possible to obtain the spatial density correlation between site occupancies $\phi_{12}=\{\langle n_1 n_2\rangle - \rho_1\rho_2\}/\bar{\rho}^2$ of the two sites behind the leading particle (Fig. 5).

A. Reduced three-particle representation

The drawback of the above approach is that it is not easy to write the transition matrix as the number of sites l is increased (number of states increases as 2^{l-1}). In the following we try to find an analytically tractable estimate for ρ_1 using an alternative reduced representation similar to Kerstein's approach [8], which yields better results for $W\sim 0$. Instead of keeping a fixed number of sites to denote a state, Kerstein chose the following infinite set of two particle states: $\{11,101,1001,10001,\cdots\}$ where the k th state has k empty sites between the leading particle (denoted by the 1 on the right) and the next particle (denoted by the 1 on the left). If there is no annihilation process—i.e., $W=0$—then these set of states is closed with respect to transitions between the states. However, as was pointed out in [9], this breaks down as soon as $W>0$. To see this let us consider the 11 state and the microscopic process in which one of the two particles gets annihilated. The resulting state depends upon the location of the third particle in the initial configuration of the lattice. I.e., one needs to go to a three-particle representation. However, the same problem occurs while considering annihilation in the 111 state. Thus, to take care of this problem which arises due to the effective non locality in transition rates by going to the moving frame attached to the leading particle one needs to make a reasonable truncation of the hierarchy. We do this first by extending the set of states to include states $\{111,1011,10011,\cdots\}$ where the rightmost 1 denotes the leading particle. Let us denote by p_k the probability of the two-particle states $10\underbrace{\ldots}_{k}01$ with k empty sites between the leading particle and the next and by q_k the probability of the three particle state $10\underbrace{\ldots}_{k}011$ with k empty sites between the second and third particles. The transition rates within these states can be written down following the procedure as in the case of fixed number of sites representation discussed in the previous section and we obtain the following rate equations for the p_k's:

$$\dot{p}_k = (2D - D\rho + W\rho)p_{k-1} + (2D+\epsilon)p_{k+1} + (q_{k-1}+q_k)W - (4D - D\rho + 3\epsilon + W\rho)p_k, \quad k \geq 2,$$

$$\dot{p}_1 = (2D - D\rho)p_0 + (2D+\epsilon)p_2 + (2q_0 + q_1)W - (4D - D\rho + 3\epsilon + W\rho)p_1,$$

$$\dot{p}_0 = (2D+\epsilon)p_1 + 2\epsilon(1-p_0) - (2D - D\rho - 2W)p_0, \quad (4)$$

where we made the approximation that ρ is the probability that the site next to the last particle in the two–or three-particle states is occupied *independent* of its distance

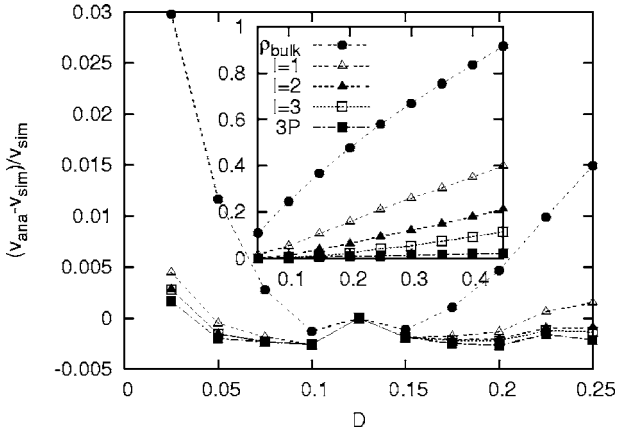

FIG. 4. Difference between front speed computed using ρ_1 from various approximations and that obtained from direct simulation as a function of D for $W=0.125$ and $W=0$ (inset). Solid squares correspond to the three-particle representation discussed in Sec. II A.

from the leading particle. We do not write the equations for q_k's as it can be shown that they can be eliminated in the steady state. To obtain the steady-state solution $\dot{p}_k=0$, following Kerstein, we make the ansatz $p_k=p_0(1-p_0)^k$ and write $\rho=Ap_0-Bp_0^2$ to take care of the ignored correlations in the ansatz in a phenomenological way. The parameters A and B are estimated as follows. We first note that for $D=W$, both the quantities ρ and p_0 equal the bulk density—namely, $\rho=p_0=\bar{\rho}=\epsilon/(\epsilon+W)$—implying $A=1+\epsilon B/(\epsilon+W)$ and thus

$$\rho=\left(1+\frac{\epsilon B}{\epsilon+W}\right)p_0-Bp_0^2. \tag{5}$$

This form also ensures that $W=0$ and $p_0=1$ imply $\rho=1$. Using ρ from Eq. (5) in Eqs. (4) (in steady state $\dot{p}_k=0$) we get the following cubic equation for p_0:

$$DB(\epsilon+W)p_0^3+(\epsilon^2+\epsilon W+\epsilon D+WD-DB\epsilon)p_0^2 +(\epsilon^2+3\epsilon W+2W^2)p_0-2\epsilon^2-2\epsilon W=0. \tag{6}$$

In order to fix B we note that for large D we expect the front to approach the mean-field limit with the speed given by $v_0=2\sqrt{2\epsilon D}$. Since in terms of p_0 the velocity is given by [from Eq. (1)] $v=\epsilon-(W-D)p_0\sim Dp_0$ for $D\gg W,\epsilon$, this implies, in this limit, $p_0=2\sqrt{2\epsilon/D}$. Substituting this expression for p_0 in Eq. (6) we obtain $B=3(\epsilon+W)/4\epsilon$. Using this expression for B in Eq. (6) one obtains $p_0=\rho_1$ implicitly through

$$D=\frac{4\epsilon(2\epsilon-\epsilon p_0^2-\epsilon p_0-2p_0W)}{(\epsilon+3\epsilon p_0+3Wp_0)p_0^2}. \tag{7}$$

The result is shown in Fig. 3 (solid square symbols marked as $3P$). We note that, although several *ad hoc* assumptions were made in arriving at Eq. (7), including using results that are strictly valid in the mean-field limit $D\to\infty$, the agreement with direct numerical results is remarkable even for the finite values of D considered. It may be noted that the three-particle representation gives best result for $W\approx 0$ (Fig. 3, inset).

B. Front diffusion coefficient D_f

In Fig. 6, we plot the front diffusion coefficient D_f as a function of D ($W=0$, $\epsilon=0.05$). The lower curve is from direct simulation and the upper one is that obtained from Eq. (1) by using the most accurate estimate of ρ_1. We see marked deviation of the values obtained from the analytic expression which implies that the simple (uncorrelated) random-walk picture of the leading particle in not quite correct. The correlated motion of the leading particle may be described as $x(t+1)-x(t)=v+\eta(t)$, where the noise term η is temporally correlated: $\langle\eta(t)\rangle=0$ and $\langle\eta(t)\eta(t')\rangle\equiv C(t-t')\neq 0$. The mean speed of the walker is v and the asymptotic diffusion coefficient is given by

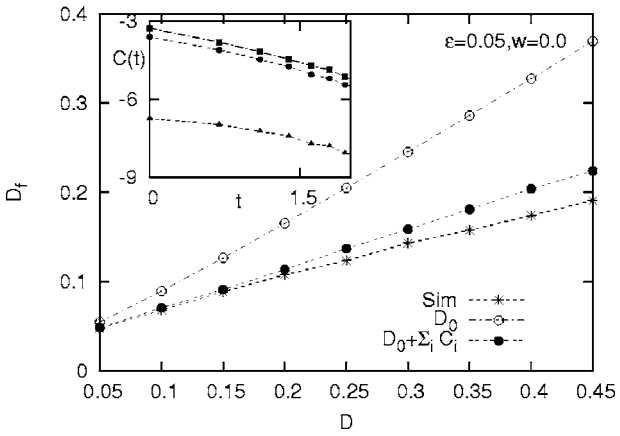

FIG. 6. Diffusion coefficient of the front for $W=0$ as a function of D. The bottom data (crosses) are the direct simulation values. The top (open circles) are the values obtained from Eq. (1) while the middle one (solid circles) represent the correlation corrected D_f. Inset: log-log plot for the correlation function $C(t)$ versus t for $D=0.45,0.35,0.05$ (from top to bottom).

$$D_f=D_0+\sum_{t=1}^{\infty}C(t), \tag{8}$$

where, $D_0=\langle\eta^2(0)\rangle$ is the diffusion coefficient given in Eq. (1) if one neglects temporal velocity correlation—i.e., $C(t)=0$ for $t>0$. Indeed, for the front under study we find that there is a quasi-long-range correlation between the successive steps of the leading particle (Fig. 6, inset). This correlation is nonpositive for all parameters (both $D>W$ as well as $D<W$) and vanishes for the special case of $D=W$. Once this correlation is taken into account the diffusion coefficient matches reasonably well with that obtained from direct simulations for the range of D studied. Preliminary fits indicate that the correlation function has the functional form $C(t)=At^{-\alpha}\exp(-t/\tau)$.

III. CONCLUSION

We have illustrated the usefulness of the leading particle picture in describing the propagation of fronts in the $A+A\leftrightarrow A$ reaction-diffusion process in the diffusion-controlled limit in one dimension. By writing the master equation in the moving frame attached to the leading particle we are able to obtain better numerical estimates for the density of the site behind the leading particle and thus the front speed v.

We have discussed two approximation schemes: the first one, which we may call as a *fixed site representation* (since it includes states corresponding to occupancy at *fixed* number of sites behind the front), is exact for $W=D$ and works well for $|W-D|\ll 1$. Here, one can systematically improve the results by including more states (i.e., increasing value of l), especially for larger $|W-D|$. In addition, this approach, in principle, allows one to compute the spatial density profile and density-density correlations away from the special point $D=W$. In the second approximation, the master equation is written in a truncated space of states with

up to a fixed number of particles behind the leading particle. Together with a product measure ansatz for site occupancy, the equations are solved self-consistently to obtain the density of site preceding the leading particle ($p_0=\rho_1$). This approach works best for $W\to 0$ for any value of D. An approach which is valid for all parameter regime is yet to be found.

Our numerical results show that the motion of the leading particle is correlated in time and this needs to be taken into account in order to get the correct diffusion coefficient. It is seen that this correction increases with increasing D (the microscopic particle diffusion constant), and thus it might play an important role in determining how the mean-field limit is achieved as $D\to\infty$.

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